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BULLETIN DU GROUPEMENT

d'informations mutuelles

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AMPERE

SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

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Contents

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Editorial

Groupement AMPERE

Dear members of the Groupement AMPERE,

an unusual year comes to an end and I would like to update you on the activities of the Groupement AMPERE. For me the highlight was clearly the online EUROMAR organized by Óscar Millet during two days in early December. On very short notice an inspiring program with 5 minutes flash talks by early-stage researchers was organized supplemented by the prize talks usually awarded at the EUROMAR. I must admit that I was a bit skeptical but the format worked very well and most of the participants stayed within their time slot. Congratulations to Óscar and his team and the scientific committee for organizing this. I really hope that in the future we will have a chance to come together at a real physical EUROMAR in Bilbao.

The EUROMAR just happened but we are already planning the EUROMAR 2021 in Portorož, Slovenia. The current plan is to have it as a hybrid meeting with physical and virtual attendees. If there is one thing, I have learned this year then it is that predictions are never correct and it is very difficult to predict the future. Therefore, we have to remain flexible and revise the planning as the situation in Europe and the rest of the world evolves. Maybe we will see some positive surprises but we cannot rely on them.

In this issue of the AMPERE Bulletin, the call for nominations for the AMPERE and Andrew Prize are published. Please submit nominations of young people for these two prizes. We rely on all of you to have a broad range of nominations from all fields of magnetic resonance.

I wish you the very best for the upcoming holiday season and the start of the new year 2021.

Best regards,

Matthias Ernst
Secretary General, Groupement AMPERE

Portrait:
Prof. Vladimir Chizhik

• Why magnetic resonance and why NMR and MRI?
In 1956, as a second-year student, I came „for company“ to the Chair of Radiophysics at the Leningrad (now St. Petersburg) University and accidentally got into the Laboratory of Radiospectroscopy, where I learned about nuclear magnetic resonance. It turned out to be my first (scientific) love, but forever!

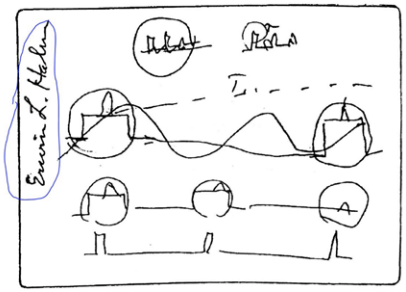
• What is your favorite frequency?
There are two frequencies to which I relate in awe: 20 MHz and 2 kHz.
In 1963, to create a pulsed NMR relaxometer (spin echo), I assembled a permanent magnet, which, after magnetization, gave a proton resonance frequency very close to 20 MHz (by accident). Two of my dissertations (PhD, 1966, and Doc. of Science, 1981) and many PhD theses of my postgraduates were done using this magnet. This magnet is still in the NMR-laboratory and is being used in educational training.
In recent years, my interests are NMR in the Earth magnetic field, where the proton resonance frequency is about 2 kHz.

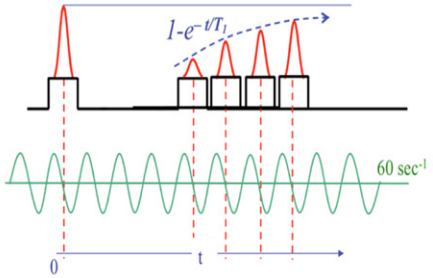
• Luckiest experiment you have ever done.
Starting in the 60s, I was able to develop a method for determining the coordination numbers of ions and the reorientation times of water molecules in ion hydration shells in solutions of strong electrolytes based on the NMR relaxation method. The final results were published: V.I. Chizhik. NMR relaxation and microstructure of aqueous electrolyte solutions. Molecular Physics. 1997, v. 90, N 4, p. 653-659; V. I. Chizhik, I. S. Podkorytov, A. P. Kaikkonen, V. I. Mikhailov. A study of solvation-shell symmetry in electrolyte solutions using quadrupolar NMR relaxation of the nuclei of monoatomic ions. J. Magn. Reson. 1996, A123, N1. P. 1-6, and are not yet criticized.
In 2014, I suggested the idea of pre-polarization of nuclei in the Earth magnetic field using a low-frequency alternating magnetic field (up to 50 Hz). The idea and its experimental confirmation were published: Vladimir I. Chizhik, Pavel A. Kupriyanov, George V. Mozzhukhin. NMR in Magnetic Field of the Earth: Pre-Polarization of

Nuclei with Alternating Magnetic Field. Applied Magnetic Resonance, 2014, 45, 641-651. doi: 10.1007/s00723-014-0543-5. I was even pleased that one of reviewers had originally written that this could not happen!

• What was the worst mistake you have made during your lab time?
I am sinless in this aspect (I think so)... Perhaps this awaits me...

• Most memorable conference story
This was in 1987 at the IX AMPERE Summer School, which took place in Russia (at that time USSR) in Novosibirsk and was attended by many outstanding scientists from around the world. During the conference dinner, the following happened. After entering the hall, Professor Erwin Hahn and his wife were undecided for a moment, and we (a small group from Russia) invited them to our table. After a few toasts, the conversation became quite relaxed, and I said to Professor E. Hahn: „I assume the discovery of the spin echo was accidental. Am I right?“ (I thought that when observing the free induction signal after a single pulse, the equipment gave off an extra pulse.) It turned out that I was only right about the „accidental“ discovery, and Professor E. Hahn took a paper napkin and started telling the story, drawing a diagram of the experiment. That time, he used adiabatic fast passage (AFP) for the measurements of spin-lattice relaxation times. It was necessary to apply slow modulation of the magnetic field and two long rf pulses for the AFP registration. Once the Professor forgot to switch on the magnetic field modulation and saw an „extra“ signal. It was the first spin echo in history! I asked for this autographed napkin as a keepsake (see below, left) and included a photocopy of it in the book „Nuclear Magnetic Relaxation“ (in Russian). Many years ago Professor E. Hahn repeated his story in a speech on the occasion of the Russell Varian Award (2004) and the picture was more beautiful, but the idea is the same (below, right: E.L. Hahn. Lille Conference talk. Journal of Magnetic Resonance. 179 (2006) 9–10).





• What do you still not understand?
1) I cannot imagine/understand the nature of the spin of nuclei or electron.
2) I consider the idea of precession cones for individual magnetic moments of nuclei (electrons) to be harmful.
3) I cannot get used to the term/understand the term (during 60 years) „spin-spin relaxation time“, since the spin-lattice relaxation is also included in this process. In my opinion, it is better to use simply „spin relaxation time“.
4) ……. (too many)

• With whom (historical person) would you like to meet?
It would be very interesting to talk to Peter the Great (the first Emperor of Russia), who founded Saint Petersburg (I have lived with this city all my life, including the Blockade of Leningrad).

• When do you get your best ideas?
I am waiting for my best idea! …

• If you had just one month time for travelling - where would you go to?
I enjoy free diving and would like to visit the Great Barrier Reef in Australia, where there are over 500 species of coral.

• Your idea of happiness.
To be among my family and we are all healthy!

Position:
Professor of the Chair of Nuclear-Physics methods of investigations , Faculty of Physics, Saint Petersburg State University
Awards:
Honored Scientist of the Russian Federation; Medal „For Services to the Fatherland“.

Homepage:
https://nsp.phys.spbu.ru/ru/

Education and so on:
Vladimir Chizhik, Professor of the Saint Petersburg State University, was born in 1937 in Leningrad (now Saint Petersburg), graduated from Leningrad University in 1959 (Faculty of Physics); 1966 – Ph. D.; 1982 – Dr. Sci. (the latter for two specialities: Radiophysics and Molecular Physics). In the Saint Petersburg (Leningrad) State University he consistently held the positions of junior researcher, senior researcher, professor. In 1993, V. Chizhik organized the new “Chair of Quantum Magnetic Phenomena” and was the Head of it during 20 years. The scientific areas of V. Chizhik are NMR in condensed matter, NMR-relaxation, microstructure of liquid systems. In 2004 V. Chizhik organized the annual International School-Conference «Magnetic resonance and its applications» (“Spinus”).

Interests: alpine skiing and free diving

First announcement

18th International School-Conference
Spinus 2021
Magnetic resonance and its applications

Saint Petersburg State University, Saint Petersburg, 29 March to 2 April, 2021

INVITATION
Welcome to the 18th International School-Conference “Spinus”. Magnetic resonance and its applications” organized by the Saint Petersburg State University from March 29 to April 2, 2021. This time the conference will be in online format (via ZOOM) due to limitations of the COVID-19 Pandemic. The goal of “Spinus” is to provide a platform to young scientists for the use of all aspects of magnetic resonance methods and techniques, as well as computational and theoretical approaches, for the solving of fundamental and applied problems in physics, chemistry, medicine and biology. The official language of the “Spinus” is English.

SCOPE
The scope of the “Spinus” Conference includes the following topics:
Modern trends in NMR, ESR and NQR, Magnetic resonance for fundamental science
Magnetic resonance imaging, Computer Modeling, NMR in the Earth magnetic field
Magnetic resonance for industry, Related areas

Extended abstracts will be published in the Book of Proceedings.
Selected papers of participants will be published in a special issue of the journal “Applied Magnetic Resonance”.

APPLICATION TO SPINUS 2021
The application for “Spinus 2021” will be available on the website spinus.spb.ru from the 4th of January, 2021.
If you were registered for “Spinus” 2018, 2019 or 2020, your account is still valid and you can create the application for Spinus-2021 in your profile.

CONFERENCE FEE
The participation fee is 2000 RUB (≈20 €) for a participant. For Russian citizens (their participation is supported by Russian funds) the participation fee is 1000 RUB. Participation fees include organization costs and conference materials.

PROCEEDINGS AND PAPER SUBMISSION
Abstracts up to 3 pages (including tables and figures) in MS Word format, according to the conference template, should be uploaded to “Spinus” website until

the 1st of March, 2021.
The abstract template is available on the site https://spinus.spb.ru/.

All accepted abstracts will be placed in the Russian Science Citation Index and will be available on the resource www.elibrary.ru

In 2021 selected papers of the participants will be published in a special issue of "Applied Magnetic Resonance" with the standard reviewing process (the journal is indexed by Web of Science and Scopus). The journal website is:
http://www.springer.com/materials/journal/723

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Vice-chairman: M. Sc. Alexandr Ievlev,
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Scientific adviser of the School-Conference "Spinus" Professor Vladimir Chizhik

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First announcement

Call for nominations
AMPERE Prize for Young Investigators 2021

The AMPERE prize has recently been redefined and is now given to a young principle researcher (a "rising star") for her/his first achievements in her/his independent career. There is no strict age limit but typically researchers below the age of forty are envisioned. The prize is given biannually.

The committee now calls for Nominations for the AMPERE Prize 2021 for a young principal investigator in the field of magnetic resonance. The prize will be presented during EUROMAR in Portoroz (Slovenia) 4-8 July 2021. The prize carries a value of € 2000.

You are kindly invited to submit nominations by e-mail to the president of the prize committee:
ampereprize@ampere-society.org

Nominations must be received by **15th February 2021** and should include the following documents:

- Nomination letter
- Curriculum vitae
- List of publications and presentations at conferences

For a list of past AMPERE Prize winners see:
www.ampere-society.org

Call for nominations
Raymond Andrew Prize 2021

In memory of Professor Dr. Raymond Andrew and to honor his pioneering work in the field of magnetic resonance, the AMPERE Group has founded the Raymond Andrew Prize. The prize is awarded to young scientists for an outstanding PhD thesis in magnetic resonance.

For the Raymond Andrew Prize 2021 the AMPERE Prize Committee is seeking your help in searching for qualified candidates who completed their dissertation during the period of 2019/2020. The prize will be presented during EUROMAR in Portoroz (Slovenia) 4-8 July 2021.

You are kindly invited to submit nominations by e-mail to:
andrewprize@ampere-society.org

Nominations must be received by **15th February 2021** and should include the following documents:

- Nomination letter
- Curriculum vitae
- List of publications and presentations at conferences
- PhD thesis in PDF

The thesis should be written in English. In exceptional cases, the thesis may also be submitted in triplicate as a hardcopy to the AMPERE Secretariat. Submissions that arrive too late will automatically be transferred to the next year. The prize committee will reconsider excellent contributions for two years in a row.

For a list of past Andrew Prize winners see:
www.ampere-society.org

Special Posterprize: Georges Menzildjian

6th International School for Young Scientists, 2020
Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics

Making binitroxides great again: a new family of water-soluble radicals for efficient dynamic nuclear polarization under MAS at very high magnetic fields.

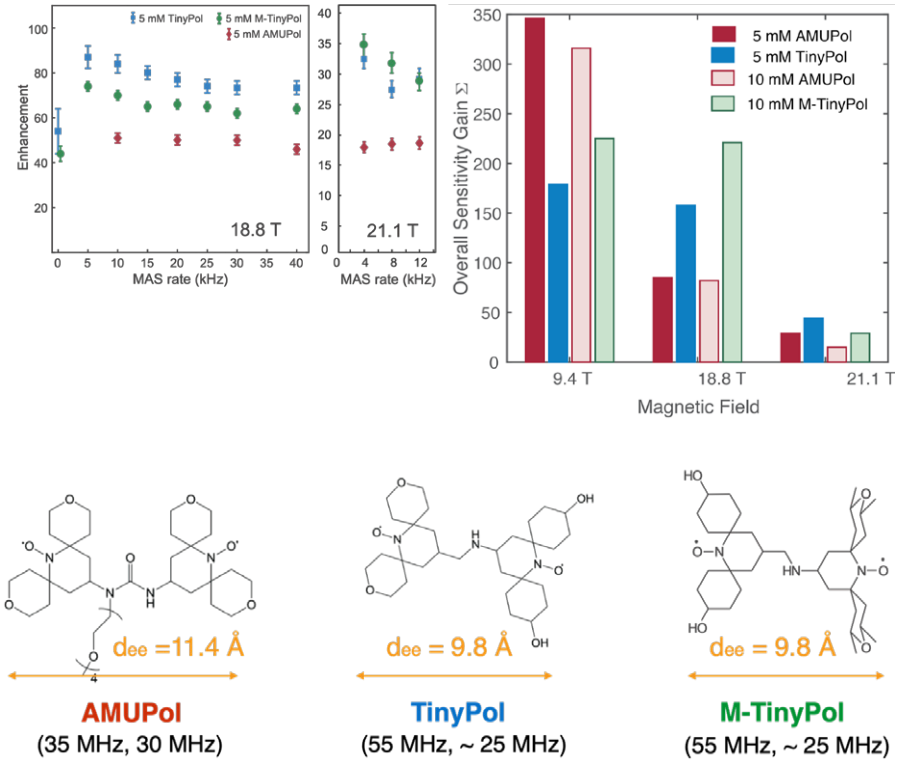
Alicia Lund (1), Gilles Casano (2), Georges Menzildjian (1), Monu Kaushik (1), Gabriele Stevanato (3), Maxim Yulikov (4), Ribal Jabbour (1), Dorothea Wisser (1), Marc Renom-Carrasco (5), Chloé Thieuleux (5), Florian Bernada (2), Hakim Karoui (2), Didier Siri (2), Melanie Rosay (6), Ivan Sergeyev (6), David Gajan (1), Moreno Lelli (7), Lyndon Emsley (3), Olivier Ouari (2) and Anne Lesage (1)
(1) Centre de RMN à Très Hauts Champs, Université de Lyon, France; (2) Aix Marseille Univ, CNRS, ICR, Marseille, France; (3) Institut des Sciences et Ingénierie Chimiques, EPFL, Switzerland ; (4) Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland; (5) Institute of Chemistry of Lyon, Laboratory C2P2 UMR 5265-CNRS-University Lyon, France ; (6) Bruker Biospin Corporation, Massachusetts, USA ; (7) Center of Magnetic Resonance (CERM), University of Florence, Sesto Fiorentino, Italy.

Dynamic nuclear polarization (DNP) has become one of the key techniques to increase the sensitivity of solid-state NMR experiments under magic angle spinning, enabling up to several 100-fold gains in signal intensity, thus opening new avenues for the characterization of challenging systems in life or materials sciences. [1,2,3]

While the standard nitroxide-based polarizing agents that are added to the sample to perform DNP, such as AMUPol [4] or TEKPol [5], routinely yield 250-fold ^{1}H enhancements at 9.4 T, their performances drop significantly at very high magnetic fields (18.8 T and above) [6]. Attempts to mitigate this decrease in efficiency were made using asymmetric binitroxides [7] or hybrid radicals [8,9], the latter being the most efficient due to the Goldilocks magnitude of their electron-electron interactions.

Based on this understanding, a new family of water-soluble binitroxide radicals, dubbed TinyPols, was designed. [10] Having a shorter tether, these radicals benefit from increased electron-electron dipolar couplings that mitigate the unfavorable DNP performances observed with binitroxides at very high magnetic fields. Enhancements up to 90 at 18.8 T and 38 at 21.1 T were obtained with the best radicals in the TinyPol series in a typical aqueous DNP matrix, offering more than a 2-fold improvement in sensitivity gain with respect to AMUPol across the whole spinning frequency range (5 to 40 kHz) accessible with a 1.3 mm LTMAS probe.

The stronger electron-electron interactions in TinyPols also mitigate the depolarization effect observed with other binitroxides. This new family of binitroxides designed for very high field DNP allows this technique to be applied to systems demanding for more resolution and sensitivity.



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[8] G. Mathies et al., Angew. Chemie – Int. Ed. 54 (40), 11770-11774 (2015) [9] D. Wisser et al., JACS 140 (41), 13340-13349 (2018)
[10] A. Lund et al., Chem. Sci. 11, 2810-2818 (2020)

Posterprize: Arnau Bertran

6th International School for Young Scientists, 2020
Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics'

Light-induced triplet-triplet electron resonance spectroscopy.

Arnau Bertran (1), Kevin B. Henbest (1), Marta De Zotti (2), Marina Gobbo (2), Christiane R. Timmel (1), Marilena Di Valentin (2) and Alice M. Bowen (3)
(1) Centre for Advanced Electron Spin Resonance and Inorganic Chemistry Laboratory, Department of Chemistry, University of Oxford, United Kingdom.
(2) Department of Chemical Sciences, University of Padova, Via Marzolo 1, 35131 Padova, Italy.
(3) National EPR Facility and Department of Chemistry, University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom.

The suitability of the porphyrin photoexcited triplet state for nanometre distance measurements by ESR Pulse Dipolar Spectroscopy was demonstrated in combination with nitroxide radicals [1]. Thanks to its non-Boltzmann population, the photoexcited triplet enhanced signal intensity when used as detection spin in PELDOR [2] and improved modulation depth when used as pump spin in LaserIMD [3]. Here we present the new technique of Light-Induced Triplet-Triplet Electron Resonance spectroscopy (LITTER), which uses photoexcited triplet states as both detection and pump spins [4]. LITTER consists in a Hahn echo sequence that moves in time with respect to two fixed laser flashes (Fig. 1 (a) and (b)). This technique has been tested in a bis-porphyrin peptide model system (1) against a single-porphyrin control (2).

A modulation is observed in 1 when Laser2 crosses the primary echo (PE), while only a slow decay attributed to triplet lifetime and T1 is observed in 2 (Fig. 1 (c)). This confirms that the effect observed in 1 is due to the intramolecular dipolar interaction between photoexcited triplet states. The form factor for 1 shows a strongly damped dipolar oscillation, which might be caused by the large conformational flexibility of the molecule. The corresponding distance distribution (Fig. 1 (e)) has a main feature within the expected values from the molecular model, showing the potential of LITTER for distance measurements between two photoexcited triplets.

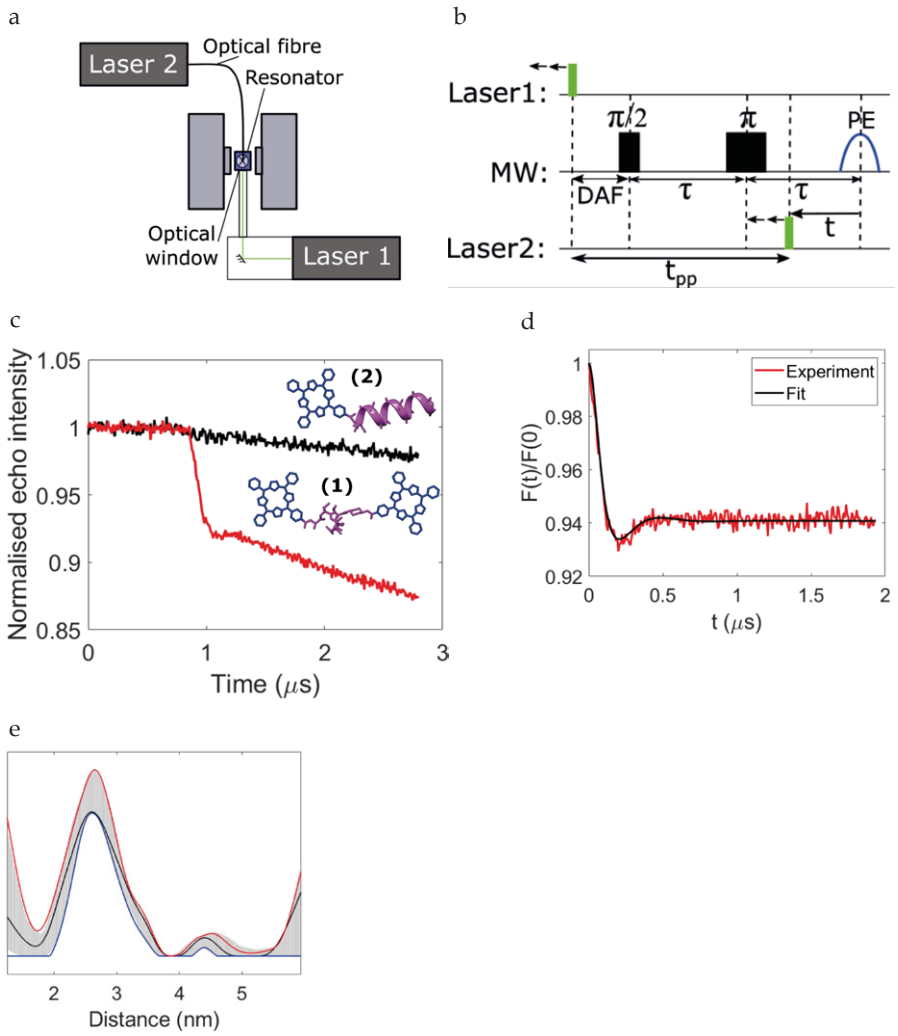

Figure 1. (a) Experimental setup and (b) pulse sequence for LITTER. (c) Normalised echo intensity traces for 1 (red) and 2 (black). (d) Background-corrected LITTER trace for 1 (red) and fit (black). (e) Corresponding distance distribution for 1 obtained using DeerAnalysis.

References:
[1] M. G. Dal Farra et al., Mol. Phys. 117, 2673-2687 (2019)
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[3] C. Hintze et al., J. Phys. Chem. Lett. 7, 2204-2209 (2016)
[4] A. Bertran et al., J. Phys. Chem. Lett. (submitted)

Posterprize: Giuseppina Magri

6th International School for Young Scientists, 2020
Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics'

Peturbed radicals in catalysis: detection of reaction intermediates in catalytic reactions by microwave perturbed EPR spectroscopy.[1]

Giuseppina Magri[1], Dr Andrea Folli[1], Dr Emma Richards[1], Prof. Adrian Porch[2] and Prof. Damien Murphy[1]
[1]School of Chemsitry, Cardiff University,
[2]School of Engineering, Cardiff University

Microwave heating continues to grow as an important enabling technology, primarily owing to the proven capability of microwaves to speed up the rate of chemical reactions. However, it is surprising that the precise molecular explanation of how microwaves heat liquids and solids remains poorly understood. Understanding this is vitally important owing to the growing use of microwave reactors for enhancing the rates of chemical reactions. This is particularly relevant in catalysis, where very large rate enhancements can be achieved using microwave heating.

Another key advantage of microwave heating for catalysis is the almost instanaeous and rapid heating of the sample. Thus, whilst microwave heating is very important in reaction rate enhancement, particularly in catalysis, our understanding of the microwave specific enhancement or heating effects are poorly understood.

The aim of this project is to develop and test a dual-mode EPR based reactor resonator. The device is built specifically to demonstrate its utility for investigating the fundamental nature of how microwave heating can influence the rate and product distribution in catalysis. This allows one to follow how reaction pathways are altered by T-jump heating and fundamentally understand how microwave specific effects lead to enhancement of photogenerated radical lifetimes and to indirectly understand how microwave heating of liquids and solids occurs. Initial focus will be on cobalt systems regarding spin cross-over events.

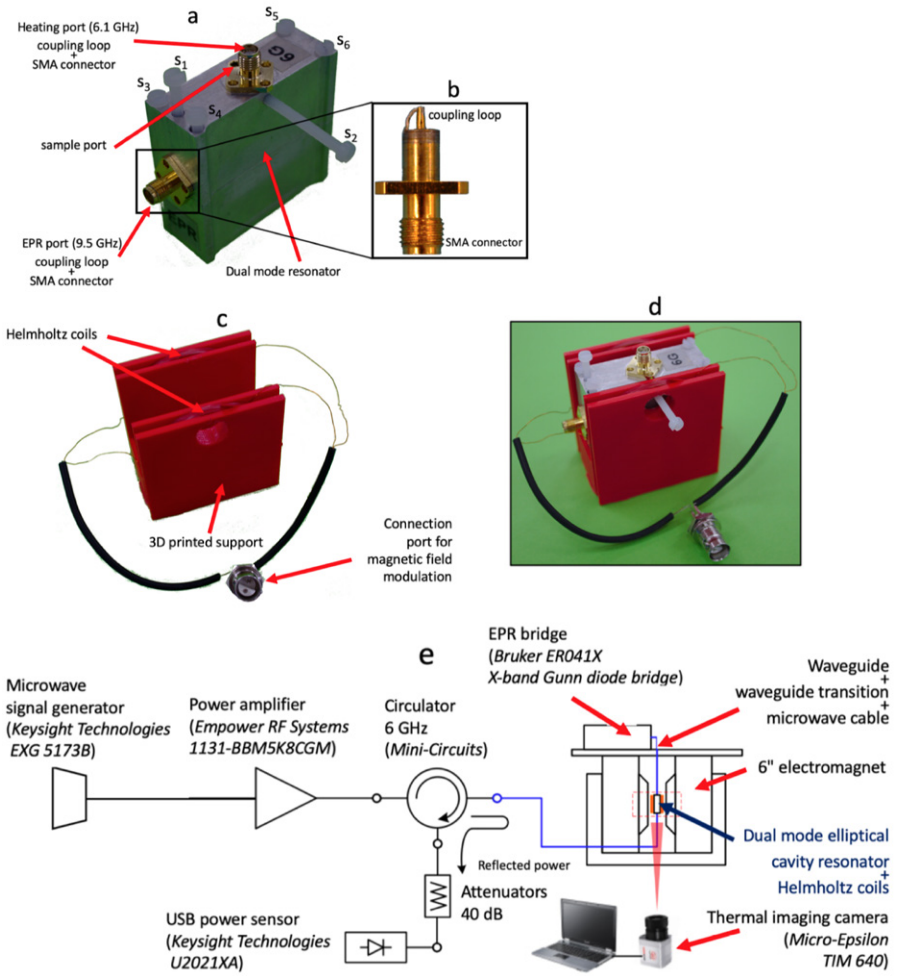

Figure 1: a) Details of Dual-Mode Cavity Resonator b) Details of Coupling Loops c) Details of Helmholtz Coils for Modulation d) Resonator Inside Support with Helmholtz Coils Shown e) Schematic Diagram of Experimental Setup for running EPR and Dielectric Heating Simultaneously.

Refereces:
1 A. Folli, H. Choi, M. Barter, J. Harari, E. Richards, D. Slocombe, A. Porch and D. M. Murphy, J. Magn. Reson., 2020, 310, 106644.

Posterprize: Natalya E. Sannikova

6th International School for Young Scientists, 2020
Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics'

Application of EPR to porphyrin-protein agents for photodynamic therapy.

Natalya E. Sannikova,[1,2] Ivan O. Timofeev,[1] Alexey S. Chubarov,[3] Natalya Sh. Lebedeva,[4] Aleksandr S. Semeikin,[5] Igor A. Kirilyuk,[6] Yuri P. Tsentalovich,[1] Matvey V. Fedin,[1] Elena G. Bagryanskaya,[6] and Olesya A. Krumkacheva,[1]
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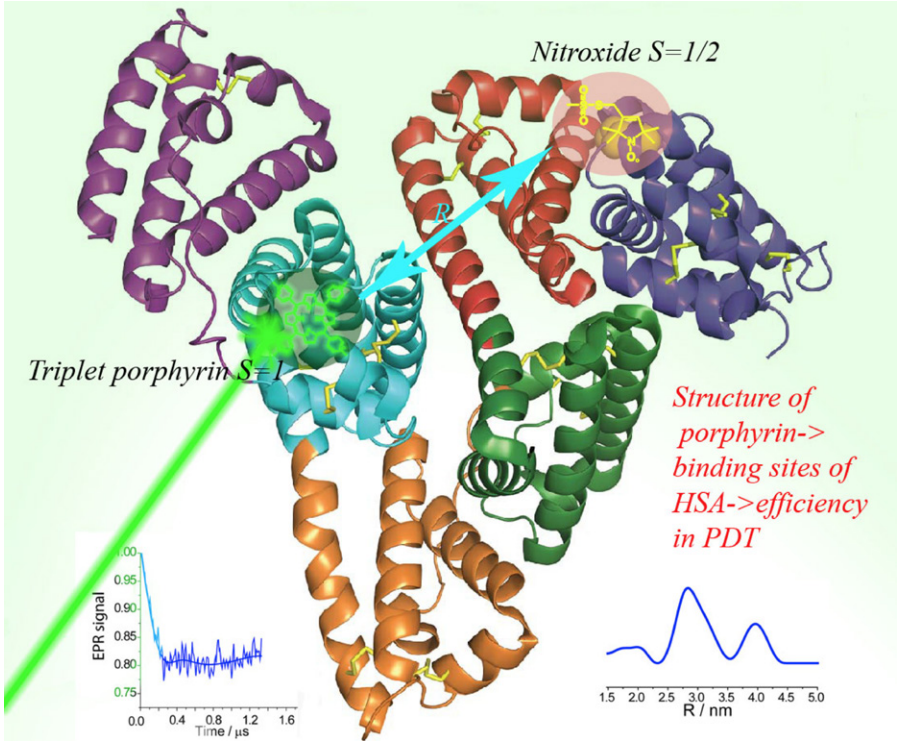
[5] Ivanovo State University of Chemistry and Technology, 153000, Ivanovo, Russia
[6] N.N. Vorozhtsov Institute of Organic Chemistry SB RAS 630090, Novosibirsk, Russia;

Recently, a new type of spin labels based on photoexcited triplet molecules was proposed for nanometer scale distance measurements by pulsed dipolar electron paramagnetic resonance (PD EPR) [1], [2]. However, such molecules are also actively used within biological complexes as photosensitizers for photodynamic therapy (PDT) of cancer. Up to date, the idea of using the photoexcited triplets simultaneously as PDT agents and as spin labels for PD EPR has never been employed. In this work [3], we demonstrate that PD EPR in conjunction with other methods provides valuable information on the structure and function of PDT candidate complexes, exemplified here with porphyrins bound to human serum albumin (HSA). Two distinct porphyrins with different properties were used: amphiphilic mesotetrakis(4-hydroxyphenyl) porphyrin (mTHPP) and water soluble cationic meso-tetra (N-methyl-4-pyridyl) porphyrin (TMPyP4); HSA was singly nitroxide-labeled to provide a second tag for PD EPR measurements. We found that TMPyP4 locates in a cavity at the center of the four-helix bundle of HSA subdomain IB, close to the interface with solvent, thus being readily accessible to oxygen. As a result, the photolysis of the complex leads to photooxidation of HSA by generated singlet oxygen and causes structural perturbation of the protein. Contrary, in case of mTHPP porphyrin, the binding occurs at the proton-rich pocket of HSA subdomain IIIA, where the access of oxygen to a photosensitizer is hindered. Structural data of PD EPR were supported by other EPR techniques, laser flash photolysis and protein photocleavage studies. Therefore, pulsed EPR on complexes of proteins with photoexcited triplets is a promising approach for gaining structural and functional insights into such PDT agents.



Acknowledgements
The experimental investigation of porphyrins and their complex with HSA was supported by Russian Science Foundation (number 20-73-10239).

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Posterprize: Fabio Santanni

6th International School for Young Scientists, 2020
Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics'

Probing nuclear-spin-economy principles in macrocyclic-based molecular spin qubits.

Fabio Santanni,[1] Andrea Albino,[1] Matteo Atzori,[2] Davide Ranieri,[1] Enrico Salvadori,[3] Mario Chiesa,[3] Lorenzo Sorace,[1] Andrea Bencini,[1] and Roberta Sessoli,[1]
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Quantum bits, or qubits, represent the fundamental units for the realization of quantum computers. Among different proposed strategies, molecular spin qubits based on transition-metal complexes, especially those containing Cu^{II} and $V^{IV}O$ [1,2], have been drawing attentions so far. They guarantee a long coherence time (T_m) over a wide range of temperatures [3], so that the superimposition state of two well defined basis states is accessible and employable for logical operations within algorithms [4].

Notwithstanding many efforts to identify the key parameters influencing the loss of coherence between qubits [5] pointed to the importance of neighboring nuclear spins, their effect in macrocyclic-based systems is still matter of debate. Indeed, while it is well established that a crucial parameter is the dimension of the nuclear spin-diffusion barrier, which can be reasonably expected in the 4 – 8 Å range [6], in Cu^{II}-phthalocyanine complex (CuPc) the hydrogen nuclei included in that non-innocent region seem not to affect the spin dynamics of the system [7].

The aim of this work is then to shed light on nuclear-spin effect on electronic spin qubits decoherence by adopting a combined experimental/theoretical study to investigate the ambiguity found in previous works, especially to unravel the effect of the peripheral hydrogen atoms in macrocyclic-based molecular spin qubits. For this purpose, we present the characterization of the coherence properties of a Cu^{II} complex obtained by using the hydrogen-free macrocyclic ligand tetrakis-thiadiazoleporphyrazine (H2TTDPz) [8], in which all the peripheral hydrogen atoms are replaced by nitrogen and sulfur nuclei [9]

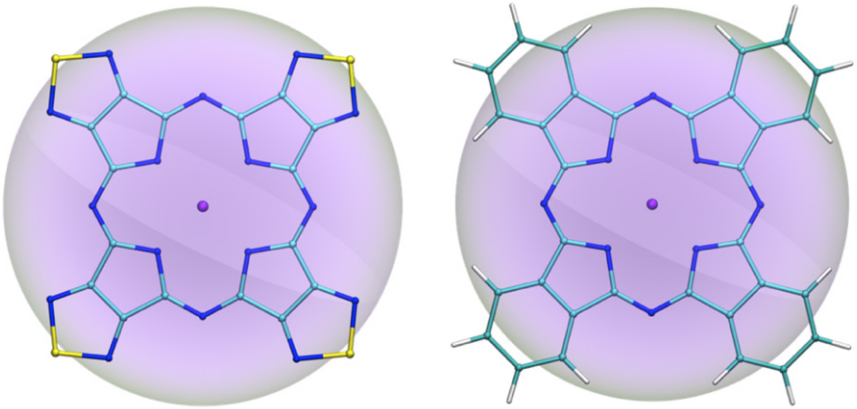

Figure 1. Molecular structures of [Cu(TTDPz)] (left) and [Cu(Pc)] (right) reported together with the expected spin diffusion barrier of 6 Å (violet sphere). Color code: C = cyan; H = white; N = blue; S = yellow; Cu = purple.

Results of the comparison between CuPc and CuTTDPz, based on pulsed EPR, ac susceptibility and *ab initio* calculations of spin-phonon coupling, allowed us to untangle the different contributions to the relaxation which are active in transition-metal complexes.

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Posterprize: Agnes E. Thorarinsdottir

6th International School for Young Scientists, 2020
Magnetic Resonance and Magnetic Phenomena in Chemical and Biological Physics'

Control of electronic spin in the design of transition metal-based Bbioresponsive magnetic resonance imaging probes.

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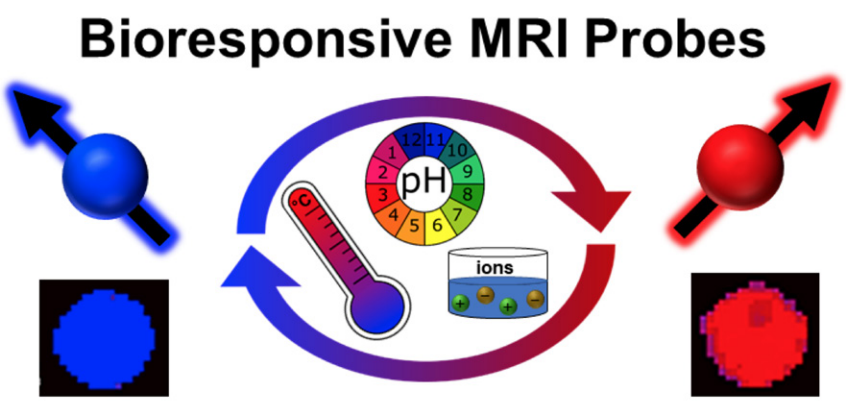
The high sensitivity of electronic spins to their surroundings renders molecules and materials featuring unpaired electrons attractive as environmental sensors. In order to successfully realize such applications, the electronic spins must be precisely controlled. Spin control using the chemical design of transition metal-based compounds is one attractive strategy toward that end owing to their exceptional synthetic tunability, high environmental responsiveness, and ease of manipulating their spin state and electronic structure.

Nevertheless, the utilization of moleculebased transition metal compounds in practical settings is scarce and further investigations are necessary to develop design principles that enable the rational synthesis of such compounds that meet society's requirements.

Herein, I report my dissertation research that focused on manipulating the electronic structure and spin state of series of transition metal complexes to design bioresponsive magnetic resonance imaging (MRI) probes, as variations in the tissue microenvironment (temperature, pH, ion concentrations, etc.) are closely associated



with a number of diseases and disorders. Specifically, spin-crossover Fe^{II} complexes were designed as temperature-responsive ^{19}F NMR chemical shift probes [1], Co^{II}_2 complexes that function as paramagnetic chemical exchange saturation transfer (PARACEST) probes were developed for the ratiometric quantitation of pH [2–4], and a mononuclear PARACEST probe that provides a ratiometric quantitation of Ca^{2+} concentration through changes in magnetic anisotropy at Co^{II} was prepared [5].

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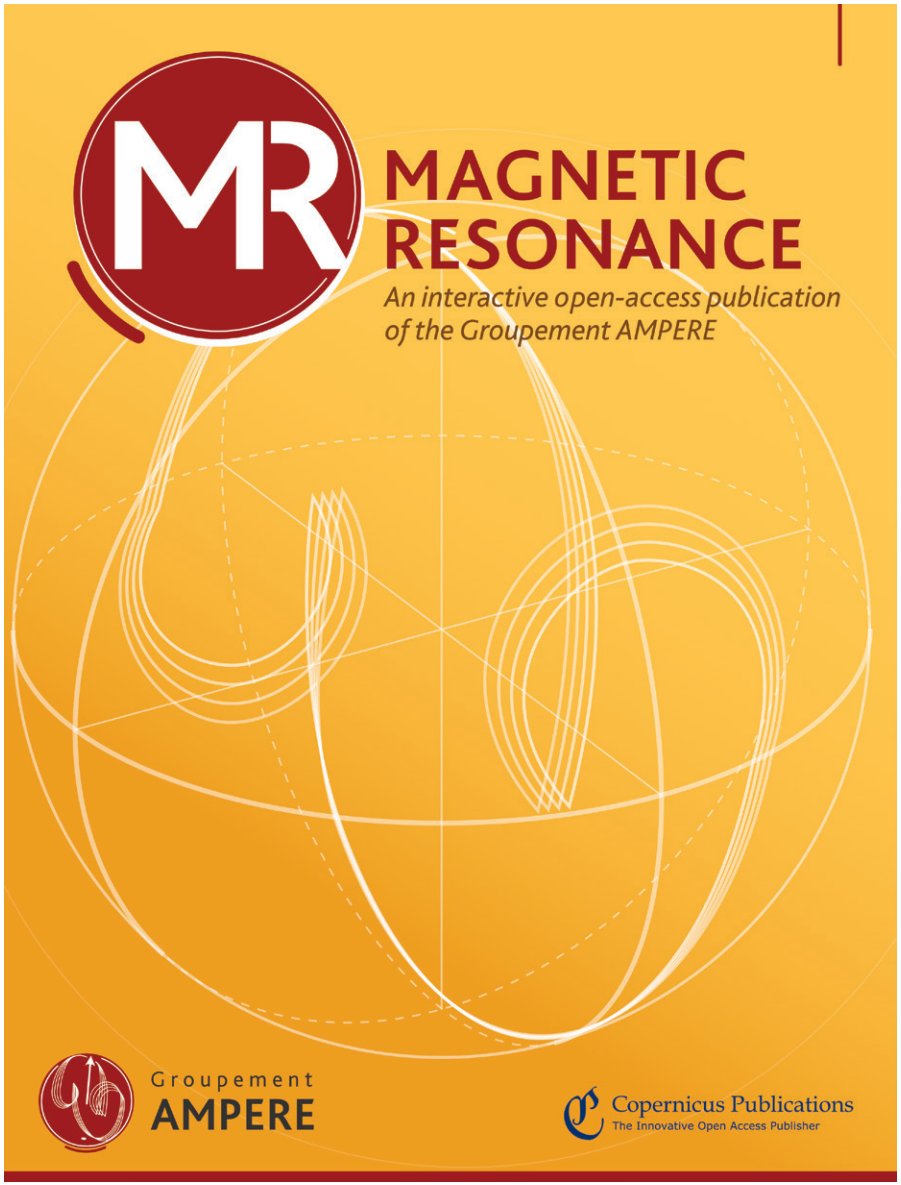

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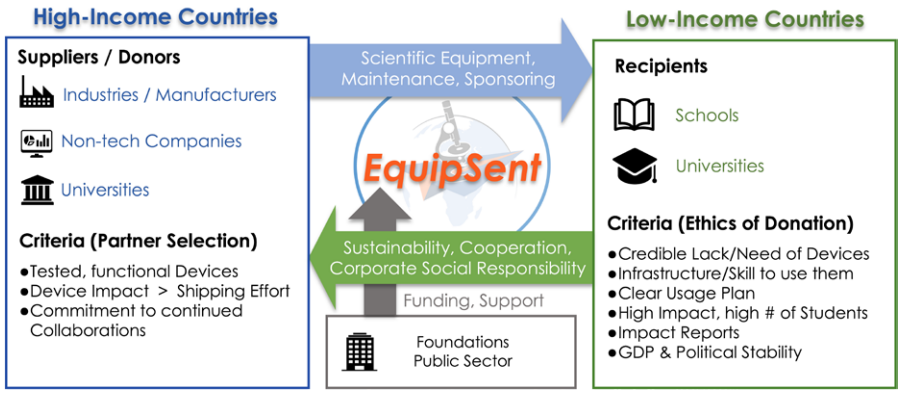

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Euromar 2021	Protorož (Slovenia)	July 4-8
16th ICMRM	Malmø (Sweden)	August 1-5
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